

1576  $C_4H_5Cl$ ED, MW, *ab initio*  
calculations (HF/4-21G)

(E)-1-Chloro-1,3-butadiene

 $C_s$   
 $H_2C=CH-CH=CHCl$ 

$r_a$	$\text{\AA}^a$	$\theta_a$	deg $^a$
C(1)=C(2)	1.340(2)	C(1)=C(2)-C(3)	122.5(4)
C(3)=C(4)	1.344(2)	C(4)=C(3)-C(2)	123.3(3)
C(2)-C(3)	1.461(3)	C(2)=C(1)-Cl	122.5(2)
C-Cl	1.728(2)		
$\Delta(C=C)^b$	0.0040 $^c$		

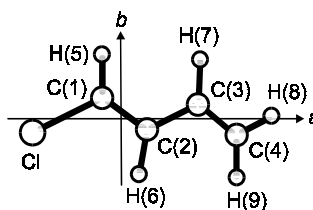
The nozzle temperature was 293 K.

 $^a$ ) Twice the estimated standard errors including the scale error. $^b$ )  $[C(1)=C(2)] - [C(3)=C(4)]$ . $^c$ ) Assumed.Gundersen, G., Thomassen, H.G., Boggs, J.E., Collins, M.L.: J. Mol. Struct. **213** (1989) 1.

MW

$r_s$	$\text{\AA}$	$\theta_s$	deg
C(1)=C(2)	1.313(10)	C(1)=C(2)-C(3)	124.1(11)
C(3)=C(4)	1.340(7)	C(4)=C(3)-C(2)	124.8(10)
C(2)-C(3)	1.439(6)	C(2)=C(1)-Cl	123.5(7)
C-Cl	1.737(4)	C(2)=C(1)-H(5)	126.1(4)
C(1)-H(5)	1.079(8)	C(1)=C(2)-H(6)	114.6(5)
C(2)-H(6)	1.129(10)	C(4)=C(3)-H(7)	119.1(6)
C(3)-H(7)	1.095(7)	C(3)=C(4)-H(8)	121.8(5)
C(4)-H(8)	1.079(9)	C(3)=C(4)-H(9)	120.1(6)
C(4)-H(9)	1.087(5)		

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$
C(1)	-0.4579	0.5416
C(2)	0.6224	-0.2208
C(3)	1.9619	0.3828
C(4)	3.0932	-0.3395
H(5)	-0.5131	1.6148
H(6)	0.4618	-1.2960
H(7)	2.0255	1.4688
H(8)	4.0663	0.1008
H(9)	3.0481	-1.4306
Cl	-2.0575	-0.1427

Cederbalk, P., Karlsson, F.: Acta Chem. Scand. Ser. A **34** (1980) 541.